

4,4'-Diaminostilbene  
621-96-5 | DTXSID2022412

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.91            | 1.08 | 0.91           | 1.08 | 0.92       | 1.00 |

Model Results

Predicted value: 1.82e-06 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.04e-01

Confidence level: 3.82e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>2-Phenylcyclohexanol</div> <div>Measured: 2.69e-06</div> <div>Predicted: 1.03e-02</div>    | <div>Image not found</div> <div>Fenuron</div> <div>Measured: 1.21e-05</div> <div>Predicted: 1.82e-05</div>    | <div>Image not found</div> <div>Naphthalene, 1,2,4,7-tetrachloro-</div> <div>Measured: 3.45e-10</div> <div>Predicted: 1.23e-05</div> |
| <div>Image not found</div> <div>1,4-Dimethylnaphthalene</div> <div>Measured: 1.63e-05</div> <div>Predicted: 6.77e-03</div> | <div>Image not found</div> <div>o-Vinyltoluene</div> <div>Measured: 1.71e-05</div> <div>Predicted: 1.93</div> |  |